

Fermi-Bose transformation for the time-dependent Lieb-Liniger gas

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Exact solutions of the Schrödinger equation describing a freely expanding Lieb-Liniger (LL) gas of delta-interacting bosons in one spatial dimension are constructed. The many-body wave function is obtained by transforming a fully antisymmetric (fermionic) time-dependent wave function which obeys the Schrödinger equation for a free gas. This transformation employs a differential Fermi-Bose mapping operator which depends on the strength of the interaction and the number of particles.

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Nonequilibrium phenomena in quantum many-body systems are among the most fundamental and intriguing phenomena in physics. One-dimensional (1D) interacting Bose gases provide a unique opportunity to study such phenomena. In some cases, the models describing these systems [1, 2, 3] allow to determine exact time-dependent solutions of the Schrödinger equation [4, 5] providing insight beyond various approximations, which is particularly important in strongly correlated regimes. These 1D systems are experimentally realized with atoms tightly confined in effectively 1D waveguides [6, 7, 8], where nonequilibrium dynamics is considerably affected by the kinematic restrictions of the geometry [8], while quantum effects are enhanced [9, 10, 11]. Today, experiments have the possibility to explore 1D Bose gases for various interaction strengths, from the Lieb-Liniger (LL) gas with finite coupling [6, 8] up to the so-called Tonks-Girardeau (TG) regime of "impenetrable-core" bosons [7, 8]. However, most theoretical studies of the exact time-dependence address the TG regime (see, e.g., Refs. [4, 12, 13, 14, 15, 16, 17, 18]). In this limit, the complex many-body problem is considerably simplified due to the Fermi-Bose mapping property [4] where dynamics follows a set of uncoupled single-particle (SP) Schrödinger equations [4]. It is therefore desirable to employ an efficient method for calculating the time-evolution of a LL gas with finite interaction strength.

In 1963, Lieb and Liniger [1] presented, on the basis of the Bethe ansatz, a solution for a homogeneous Bose gas with (repulsive) δ -function interactions, for arbitrary interaction strength c ; periodic boundary conditions were imposed. This system was analyzed by McGuire on an infinite line with attractive interactions [3]. The renewed interest in 1D Bose gases stimulated recent studies of static LL wave functions [19, 20, 21] including a LL gas in box confinement [21]. Besides the wave functions, the correlations of a LL system with finite coupling [22, 23, 24, 25, 26, 27, 28, 29, 30, 31] provide a link to many observables and were analyzed by using various techniques, including the inverse scattering method [24, 25, 30, 31], $1/c$ expansions [23] relying on

the analytic results in the TG regime [32], and numerical Quantum Monte Carlo techniques [28]. Regarding dynamics, a full numerical study of the irregular dynamics in a mesoscopic LL system was presented in [33]. In Ref. [5], Girardeau has shown that phase imprinting by light pulses conserves the so-called cusp condition imposed by the interactions on the LL wave functions, and suggested to use time-evolving SP wave functions to analyze the subsequent dynamics. However, as pointed out in Ref. [5], the presented scheme does not obey the cusp condition during the evolution which limits its validity. This situation can be remedied by using an ansatz which obeys the cusp condition at all times by construction [24, 34].

Here we construct exact solutions for the freely expanding LL gas with localized initial density distribution. This can be achieved by differentiating a fully antisymmetric (fermionic) time-dependent wave function, which obeys the Schrödinger equation for a free Fermi gas [34]; the employed differential operator depends on the interaction strength c and the number of particles. When $c \rightarrow \infty$, the scheme reduces to Girardeau's time-dependent Fermi-Bose mapping [4], valid for "impenetrable-core" bosons.

We consider the dynamics of N indistinguishable δ -interacting bosons in a 1D geometry [1]. The Schrödinger equation for this system is

$$i \frac{\partial \psi_B}{\partial t} = - \sum_{i=1}^N \frac{\partial^2 \psi_B}{\partial x_i^2} + \sum_{1 \leq i < j \leq N} 2c \delta(x_i - x_j) \psi_B, \quad (1)$$

where $\psi_B(x_1, \dots, x_N, t)$ is the many-body wave function, and c quantifies the strength of the interaction (for connection to physical units see, e.g., [5]). The x -space is infinite (we do not impose any boundary conditions), which corresponds to a number of interesting experimental situations where the gas is initially localized within a certain region of space and then allowed to freely evolve. This is relevant for free expansion [13, 14, 15, 16] or interference of two initially separated clouds during such expansion [12], etc. Due to the Bose symmetry, it is sufficient to express the wave function ψ_B in a single permutation sec-

tor of the configuration space, $R_1 : x_1 < x_2 < \dots < x_N$. Within R_1 , ψ_B obeys

$$i\partial\psi_B/\partial t = -\sum_{i=1}^N \partial^2\psi_B/\partial x_i^2, \quad (2)$$

while interactions impose boundary conditions at the borders of R_1 [1]:

$$\left[1 - \frac{1}{c} \left(\frac{\partial}{\partial x_{j+1}} - \frac{\partial}{\partial x_j} \right)\right]_{x_{j+1}=x_j} \psi_B = 0. \quad (3)$$

This constraint creates a cusp in the many-body wave function when two particles touch, which should be present at any time during the dynamics.

In the TG limit (i.e., when $c \rightarrow \infty$) the cusp condition is $\psi_B(x_1, \dots, x_j, x_{j+1}, \dots, x_N, t)|_{x_{j+1}=x_j} = 0$ [2, 4], which is trivially satisfied by an antisymmetric fermionic wave function $\psi_F(x_1, \dots, x_N, t)$; thus $\psi_B = \psi_F$ within R_1 , which is the famous Fermi-Bose mapping [2, 4]. In many physically interesting cases, ψ_F can be constructed as a Slater determinant

$$\psi_F(x_1, \dots, x_N, t) = (N!)^{-\frac{1}{2}} \det[\phi_m(x_j, t)]_{m,j=1}^N. \quad (4)$$

Since $\psi_B = \psi_F$ within R_1 , ψ_F must obey $i\partial\psi_F/\partial t = -\sum_{j=1}^N \partial^2\psi_F/\partial x_j^2$, which implies that the (orthonormal) SP wave functions $\phi_m(x_j, t)$ evolve according to

$$i\partial\phi_m/\partial t = -\partial^2\phi_m/\partial x^2; \quad (5)$$

$m = 1, \dots, N$. Thus, in the TG limit, the complexity of the many-body dynamics is reduced to solving a simple set of uncoupled SP equations, while the interaction constraint (3) is satisfied by the Fermi-Bose construction.

The simplicity and success of this idea motivates us to choose an ansatz which automatically satisfies constraint (3) for any finite c [24, 34]. For this, define a differential operator

$$\hat{O} = \prod_{1 \leq i < j \leq N} \hat{B}_{ij}, \quad (6)$$

where \hat{B}_{ij} stands for

$$\hat{B}_{ij} = \left[1 + \frac{1}{c} \left(\frac{\partial}{\partial x_j} - \frac{\partial}{\partial x_i} \right)\right]. \quad (7)$$

It can be shown that the wave function

$$\psi_B = \mathcal{N}_c \hat{O} \psi_F \text{ (inside } R_1), \quad (8)$$

where \mathcal{N}_c is a normalization constant, obeys the cusp condition (3) by construction [24, 34]: Consider an auxiliary wave function

$$\begin{aligned} \psi_{\text{AUX}}(x_1, \dots, x_N, t) &= \hat{B}_{j+1,j} \hat{O} \psi_F \\ &= \hat{B}_{j+1,j} \hat{B}_{j,j+1} \hat{O}'_{j,j+1} \psi_F, \end{aligned} \quad (9)$$

where the primed operator $\hat{O}'_{j,j+1} = \hat{O}/\hat{B}_{j,j+1}$ omits the factor $\hat{B}_{j,j+1}$ as compared to \hat{O} . The auxiliary function can be written as

$$\psi_{\text{AUX}} = \left[1 - \frac{1}{c^2} \left(\frac{\partial}{\partial x_{j+1}} - \frac{\partial}{\partial x_j} \right)^2\right] \hat{O}'_{j,j+1} \psi_F. \quad (10)$$

It is straightforward to verify that the operator $\hat{B}_{j+1,j} \hat{B}_{j,j+1} \hat{O}'_{j,j+1}$ in front of ψ_F is invariant under the exchange of x_j and x_{j+1} [24]. On the other hand, the fermionic wave function ψ_F is antisymmetric with respect to the interchange of x_j and x_{j+1} . Thus, $\psi_{\text{AUX}}(x_1, \dots, x_j, x_{j+1}, \dots, x_N, t)$ is antisymmetric with respect to the interchange of x_j and x_{j+1} , which leads to [24, 34]

$$\psi_{\text{AUX}}(x_1, \dots, x_j, x_{j+1}, \dots, x_N, t)|_{x_{j+1}=x_j} = 0. \quad (11)$$

This is fully equivalent to the cusp condition (3), $\hat{B}_{j+1,j} \psi_B|_{x_{j+1}=x_j} = 0$ [24, 34]. Thus, the wave function (8) obeys constraint (3) by construction.

In order to exactly describe the dynamics of LL gases, the wave function (8) should also obey Eq. (2) inside R_1 . From the commutators $[\partial^2/\partial x_j^2, \hat{O}] = 0$ and $[i\partial/\partial t, \hat{O}] = 0$ it follows that if ψ_F is given by Eq. (4) and the $\phi_m(x_j, t)$ obey Eq. (5), then ψ_B obeys Eq. (2). Note that for $c \rightarrow \infty$, one recovers Girardeau's Fermi-Bose mapping [2, 4], i.e., $\hat{O} = 1$.

Let us utilize this formalism to describe the dynamics of a freely expanding LL gas. Suppose that for $t < 0$ the system is confined by an external potential $V(x)$ and is in its ground state, before at $t = 0$ the potential is suddenly switched off. In order to find the exact form of the initial condition, we have to solve the static Schrödinger equation for the LL gas in the potential $V(x)$. By using the above formalism, we express the initial state as $\psi_{B0} = \mathcal{N}_c \hat{O} \psi_{F0}$, which should (within R_1) obey $\sum_j H_j \psi_{B0} = E_{B0} \psi_{B0}$ or, equivalently,

$$\hat{O} \sum_j H_j \psi_{F0} - [\hat{O}, \sum_j H_j] \psi_{F0} = \hat{O} E_{B0} \psi_{F0}. \quad (12)$$

Here, E_{B0} is the ground-state energy, and $H_j = -\partial^2/\partial x_j^2 + V(x_j)$ is the SP hamiltonian. Eq. (12) shows that, due to the nonvanishing commutator $[\hat{O}, \sum_j H_j] = [\hat{O}, \sum_j V(x_j)]$, operating with \hat{O} on the fermionic ground state in the trap does not give the bosonic ground state. However, for sufficiently strong interactions and/or weak and slowly varying potentials, we can approximate $[\hat{O}, \sum_j V(x_j)] \approx 0$. In the TG limit, the commutator vanishes identically. Thus, for sufficiently strong interactions, the ground state is approximated by $\psi_{B0} = \mathcal{N}_c \hat{O} \det[\phi_m(x_j, 0)]_{m,j=1}^N / \sqrt{N!}$, where $\phi_m(x_j, 0)$ is the m th eigenstate of the SP hamiltonian.

In what follows we study free expansion from such an initial condition, which describes a LL gas with a

localized density distribution. Even though ψ_{B0} can not be interpreted as a ground state for weak interactions, the free expansion from ψ_{B0} is calculated exactly for all values of c . We illustrate the properties of $\psi_{B0} = \mathcal{N}_c \hat{O} \det[\phi_m(x_j, 0)]_{m,j=1}^N / \sqrt{N!}$ for the harmonic potential $V(x) = \nu^2 x^2/4$, with $\nu = 2$. Fig. 1 (left column) displays the section $|\psi_{B0}(0, x_2, x_3)|^2$ of the probability density, for $N = 3$ particles and three values of c . We clearly see that, as the interaction strength increases, the initial state becomes more correlated. Given that one particle is located at zero, for $c = 1$ there is a considerable probability that the other two particles are to the left or to the right of the first one, i.e., their positions are weakly correlated with that of the first particle. However, for larger c , if one particle is at zero, it is more likely that the other two particles are on opposite sides of the first one, and their distance grows with increasing interaction strength.

When the harmonic potential is turned off, the evolution of the SP states $\phi_m(x, t)$ is known exactly (see, e.g., Ref. [15]): $\phi_m(x, t) = \phi_m(x/b(t), 0) \exp[ix^2 b'(t)/(4b(t)) - iE_m \tau(t)]/\sqrt{b(t)}$, where E_m is the energy of the m th SP eigenstate $\phi_m(x, 0)$, $b(t) = \sqrt{1 + t^2 \nu^2}$, and $\tau(t) = \arctan(\nu t)/\nu$. We can make use of the expression for the ground state of a TG gas in harmonic confinement [35] to calculate ψ_{F0} . Employing Eq. 8, the evolution of the many-body wave function ψ_B can then be formally expressed (within R_1) as

$$\psi_B = \mathcal{N}(c, \nu, N) b(t)^{-\frac{N^2}{2}} e^{-i\frac{N^2 \nu}{2} \tau(t)} \hat{O} e^{-\frac{\nu - i\nu^2 t}{4} \sum_{j=1}^N [x_j/b(t)]^2} \prod_{1 \leq i < j \leq N} (x_j - x_i), \quad (13)$$

where $\mathcal{N}(c, \nu, N)$ is a normalization constant, evaluating to $\mathcal{N} = 1$ for $c \rightarrow \infty$. The action of the operator \hat{O} yields lengthy expressions already for a few particles, and particular examples will be given elsewhere. The asymptotic form of Eq. (13) is given by $\lim_{t \rightarrow \infty} \psi_B/\psi_F \propto \{\hat{O} \prod_{1 \leq i < j \leq N} (x_j - x_i)\} / \prod_{1 \leq i < j \leq N} (x_j - x_i)$. Although Eq. (13) provides an exact wave function for the time-dependent LL gas, it is desirable to calculate the evolution of observables such as the SP density $\rho(x, t) = N \int dx_2 \dots dx_N |\psi_B(x, x_2, \dots, x_N, t)|^2$. This task is complicated by the many-fold integral. However, we can find the evolution of $\rho(x, t)$ numerically for small numbers of particles. Fig. 1 (right column) displays the evolution of the SP density for three different values of c . For larger c , the initial SP density exhibits typical TG-fermionic properties, characterized by N small separated humps [4, 12]. For all values of c , the SP density acquires such humps during free expansion indicating that the system becomes more correlated in time, which is in accord with the fact that the LL gas becomes strongly correlated for lower densities [1].

Even though the employed approach is valid at any interaction strength, it is particularly useful for the

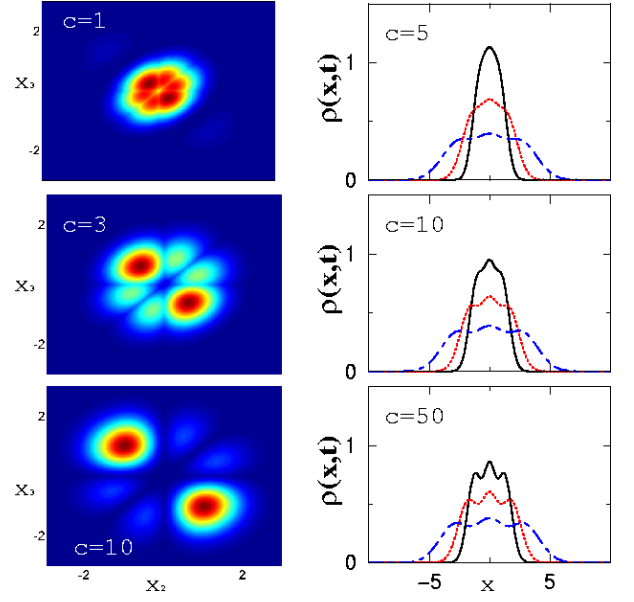


FIG. 1: (color online) The correlation properties of the initial state and the evolution of the SP density for various interaction strengths, for $N = 3$ particles. (Left column) The probability density $|\psi_{B0}(0, x_2, x_3)|^2$ for $c = 1, 3, 10$. (Right column) The SP density at $t = 0$ (black solid line), $t = 0.5$ (red dotted line), and $t = 1$ (blue dot-dashed line), for $c = 5, 10, 50$.

strongly interacting gas: First, the operator \hat{O} can be hierarchically organized into orders $1/c^k$, $\hat{O} = 1 + \sum_{k=1}^{N(N-1)/2} c^{-k} \hat{O}_k$. By keeping the terms of order $1/c$, we obtain the first-order correction to the TG gas. In this approximation, the form of the operator is considerably simplified, $\hat{O} \approx 1 + c^{-1} \hat{O}_1$, where $\hat{O}_1 = \sum_{k=1}^N (2k - N - 1) \partial/\partial x_k$. The wave function reads, within R_1 ,

$$\psi_B = \psi_F + \sum_{k=1}^N \frac{2k - N - 1}{c \sqrt{N!}} \det[A_{mj}^k]_{m,j=1}^N, \quad (14)$$

where $A_{mj}^k = \phi_m(x_j, t)$ for $j \neq k$, and $A_{mk}^k = \partial \phi_m(x_k, t)/\partial x_k$. The numerical calculation of the wave function (14) is not a difficult task even for a fairly large numbers of particles. Second, in this regime, $[\hat{O}, \sum_j H_j] = [\hat{O}, \sum_j V(x_j)] \approx 0$ is a reasonable approximation. For example, with $\hat{O} \approx 1 + c^{-1} \hat{O}_1$ and $V(x) = \nu^2 x^2/4$, $[\hat{O}, \sum_j V(x_j)]$ is of order $\nu^2/4c$, i.e., for $\nu^2 \leq 1/c$ the commutator is of order $1/c^2$ or less. Thus, the approach can be used to characterize time-dependent and static LL gases in various trapping potentials in the strongly correlated regime, but below the TG gas limit.

For completeness, let us briefly discuss time-evolving states ψ_B with periodic boundary conditions as in Ref. [1]. Any time-evolving state ψ_B can be written as a superposition of eigenstates $\psi_{LL, \xi}(x_1, \dots, x_N)$, where ξ denotes all quantum numbers necessary to describe one eigenstate. LL eigenstates can be written as $\psi_{LL, \xi} =$

$\hat{O}\mathcal{N}_\xi \det[e^{ik_mx_j}]_{m,j=1}^N$ [24, 34]. If periodic boundary conditions are imposed as in Ref. [1], the quasimomenta k_j must obey a set of coupled transcendental equations and depend on c [1, 20]. Time-evolving states ψ_B can be written as a superposition of LL eigenstates

$$\psi_B = \hat{O} \sum_{\xi} \mathcal{N}_\xi b(\xi) \det[e^{ik_mx_j}]_{m,j=1}^N e^{-iE_\xi t}, \quad (15)$$

where the coefficients $b(\xi)$ are fixed by the initial conditions. These coefficient are in practice hard to calculate given the initial state due to the many-fold integrations that need to be performed.

It should be emphasized that the Fermi-Bose transformation employed here differs from the fermion-boson duality discussed by Cheon and Shigehara [36] (see also [37]), because it transforms a *noninteracting* fermionic wave function into a wave function describing LL gas. Using Ref. [36] it can be shown that the approach used here can also be applied to construct wave functions for a time-dependent Fermi gas with finite-strength interactions.

In conclusion, we have constructed exact solutions for the freely expanding LL gas with localized initial density distribution. Wave functions are obtained by differentiating a fully antisymmetric (fermionic) time-dependent wave function, which obeys the Schrödinger equation for a free Fermi gas. For a number of physically interesting situations (e.g., free expansion), by using the operator \hat{O} , the state of the system can be derived from N SP time-dependent states, as anticipated in Ref. [5]. The construction of LL wave functions for various external potentials $V(x)$, and the derivation of correlation functions within the employed formalism is the subject of ongoing work.

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